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Abstract
Solute additions are commonly used to stabilize nanocrystalline materials against grain growth, and can simultaneously enhance the strength of the material by impeding dislocation emission from the grain boundaries. In this study we demonstrate using molecular dynamics (MD) simulations that the effect of solutes on dislocation nucleation depends on the distribution of solutes at the grain boundary, and can vary dramatically depending on the solute type. Solutes with a *smaller* positive size mismatch to the host can be more effective in suppressing dislocation emission from grain boundaries than others that have *larger* mismatch. In particular, although Ag solutes have a smaller misfit with Cu than Zr solutes, the effect of Ag on the dislocation nucleation from grain boundaries in Cu can be larger than the corresponding effect of Zr. These findings are relevant to the search for optimal solute additions, which can strengthen a nanocrytalline material by suppressing the nucleation of dislocation slip from grain boundaries, while stabilizing it against grain growth.

Keywords
Solute segregation at grain boundaries, Dislocation nucleation, Yield stress, Monte Carlo simulation, Molecular dynamics simulation

Disciplines
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Effects of Ag and Zr solutes on dislocation emission from Σ11(332)[110] symmetric tilt grain boundaries in Cu: bigger is not always better

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Solute additions are commonly used to stabilize nanocrystalline materials against grain growth, and can simultaneously enhance the strength of the material by impeding dislocation emission from the grain boundaries. In this study we demonstrate using molecular dynamics (MD) simulations that the effect of solutes on dislocation nucleation depends on the distribution of solutes at the grain boundary, and can vary dramatically depending on the solute type. Solutes with a *smaller* positive size mismatch to the host can be more effective in suppressing dislocation emission from grain boundaries than others that have *larger* mismatch. In particular, although Ag solutes have a smaller misfit with Cu than Zr solutes, the effect of Ag on the dislocation nucleation from grain boundaries in Cu can be larger than the corresponding effect of Zr. These findings are relevant to the search for optimal solute additions, which can strengthen a nanocrytalline material by suppressing the nucleation of dislocation slip from grain boundaries, while stabilizing it against grain growth.

Keywords: solute segregation at grain boundaries, dislocation nucleation, yield stress, Monte Carlo simulation, molecular dynamics simulation.

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1. Introduction

The grain sizes of polycrystalline materials strongly affect their plastic deformation behavior (Hahn and Meyers, 2015) and very significant strengthening can be achieved by reducing grain size into the range of about 15-100 nm (Armstrong, 2014) where dislocation generation is dominated by grain boundaries rather than intra-granular sources (Chen et al., 2012; Khan and Liu, 2016; Prakash et al., 2017; Yang et al., 2006; Zhang et al., 2017). Smaller grain sizes (<15 nm) can result in softening due to a crossover from dislocation-mediated plasticity to grain boundary (GB) mediated plasticity promoted by grain boundary sliding (Ovid'ko and Sheinerman, 2017) and grain rotation (Argon and Yip, 2006; Schiotz and Jacobsen, 2003). Using the strength of nanocrystalline materials in engineering applications is restricted, however, because they are thermally unstable. Significant coarsening occurs even at relatively low temperatures, resulting in loss of strength. The addition of low-solubility alloying elements, which tend to segregate at grain boundaries (Yu and Shen, 2016), can stabilize a nanocrystalline material against grain growth (Chookajorn et al., 2012; Darling et al., 2014; Frolov et al., 2012) and also suppress grain boundary mediated plasticity mechanisms (Millett et al., 2006). Since dislocation emission from grain boundaries is a key deformation mechanism over a wide range of grain sizes, the opportunity arises to utilize a single solute to suppress *both* grain growth *and* the nucleation of the dislocations from grain boundaries (Borovikov et al., 2017), resulting in a stable, high-strength nanocrystalline material. In this study, we seek to illuminate the factors that make solute atoms effective at suppressing dislocation nucleation from grain boundaries.

We have previously demonstrated that solute atoms can have a very strong effect on the process of dislocation nucleation from grain boundaries (Borovikov et al., 2017): a significant increase in the yield stress results from both oversized (Ag in Cu) and undersized (Cu in Ag) solutes. It has also been argued that substitutional solutes with larger size mismatches increase the yield strength more effectively than those with smaller ones (Ozerinc et al., 2012; Vo et al., 2011). Comparison of the data obtained in (Borovikov et al., 2017) and (Ozerinc et al., 2012; Vo et al., 2011) leads to the conclusion that the atomic mismatch can not be the only factor governing the effect of the solute atoms. In order to clarify this, we now report on new molecular dynamics (MD) simulations of the effects of Ag and Zr solutes on dislocation nucleation from $\Sigma 11(332)[110]$ symmetric tilt grain boundaries (STGBs) in Cu. We demonstrate that the effect of solutes strongly depends on their segregation pattern and solute atoms with a *smaller* positive size mismatch (Ag in Cu) can suppress the nucleation of dislocations from the grain boundary more effectively than solute atoms with a larger one (Zr in Cu).

The rest of the paper is organized as follows. First, we will describe the simulation geometry, computational methods and the selection of a suitable semi-empirical potential of the interatomic interactions. Next, we will discuss the differences in the segregation patterns of the Ag and Zr solutes at the GB we considered in this study. Finally, we will show how these differences affect the dislocation nucleation from the GB.

2. Simulation geometry and interatomic interaction

The effect of two solutes in Cu were considered: Ag and Zr. Both solutes have larger

atomic radii (144 pm for Ag and 160 pm for Zr) than Cu (128 pm). Since MD simulations of plastic deformation require large simulation cells containing at least tens of thousands atoms and long simulation times, employing semi-empirical potentials is the only reasonable option. We have already studied the effect of Ag solutes on dislocation nucleation from GB in Cu (Borovikov et al., 2017) using the Cu-Ag embedded atom method (EAM) potential (Daw and Baskes, 1984) developed in (Williams et al., 2006). Ideally we would like to use a Cu-Zr semi-empirical potential developed in the exactly the same way. Unfortunately, there is no such a potential in the literature. Instead, there is a Finnis-Sinclair (FS) potential (Finnis and Sinclair, 1984) for the Cu-Zr alloys developed in (Mendelev et al., 2009). However, the Cu potential from (Daw and Baskes, 1984) leads to 2.8 meV/Å^2 and 10.1 meV/Å^2 for the stable and unstable stacking fault energies, respectively, and the Cu potential from (Mendelev et al., 2009) leads to 2.4 meV/Å^2 and 16.6 meV/Å^2, and the stable and unstable stacking fault energies both affect dislocation nucleation from GBs (Borovikov et al., 2016). To compare the effects of Ag and Zr additions on dislocation nucleation in Cu we need potentials that give similar Cu properties in the absence of solutes. This precondition will be met if the Cu potential in the Cu-Zr potential from (Mendelev et al., 2009) is replaced by the MCu31 potential developed in (Borovikov et al., 2016). This potential leads to 2.8 meV/Å^2 and 10.1 meV/Å^2 for the stable and unstable stacking fault energies, respectively, as does the Cu-Ag potential.

To confirm that the selected Cu potentials lead to similar behavior during plastic deformation in pure Cu, we performed MD simulations at T=300 K utilizing a simple bi-crystal geometry in which the emission of dislocations from a grain boundary is the only active mechanism of plastic deformation. The simulation cell has two Σ11(332)[110] symmetric tilt grain boundaries which contain the structural units designated as type E (Rittner and Seidman, 1996). Our choice of this GB results from the observation that symmetric tilt grain boundaries within the <110> family, which contain the E structural units, are able to emit dislocations under lower applied stresses than other grain boundaries (Spearot et al., 2007b; Tschopp et al., 2007). All simulations were carried out using the LAMMPS simulation package (Plimpton, 1995) and the visualization of the simulation snapshots was performed using the OVITO package (Stukowski, 2010). The simulation cell is shown in Fig. 1. Periodic boundary conditions were used in all three directions. The simulation cell size was sufficiently large in all three directions (greater than 16 nm in the directions parallel to GB plane, and greater than 32 nm in the direction normal to GB plane) to minimize the effect of periodic boundary conditions on dislocation nucleation (Spearot et al., 2007a; Spearot et al., 2007b). Uniaxial tensile loading simulations were carried out with a constant engineering strain rate of 10^8 s^{-1} applied in the z direction (normal to the grain boundary plane), while the stresses in the other two directions were held at zero. Other details of the simulation were identical to those used in (Borovikov et al., 2017).

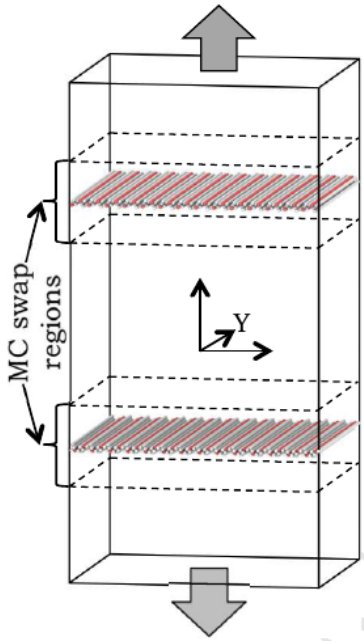

Figure 1. The bi-crystal simulation system; the MC swap regions are indicated by dashed lines. The arrows indicate the direction of the applied deformation.

At the onset of deformation the stress gradually increases with increasing applied strain and eventually drops abruptly when the first dislocation is emitted (see Fig. 2). The value of this peak stress is taken as the effective yield stress. Figure 2 shows the data obtained for the three Cu potentials discussed above. The Cu potential taken from the Cu-Ag potential and MCu31 indeed lead to similar curves. The Cu potential taken from the Cu-Zr potential leads to a higher value of the yield stress resulting from the larger value of the unstable staking fault energy as discussed in (Borovikov et al., 2016).

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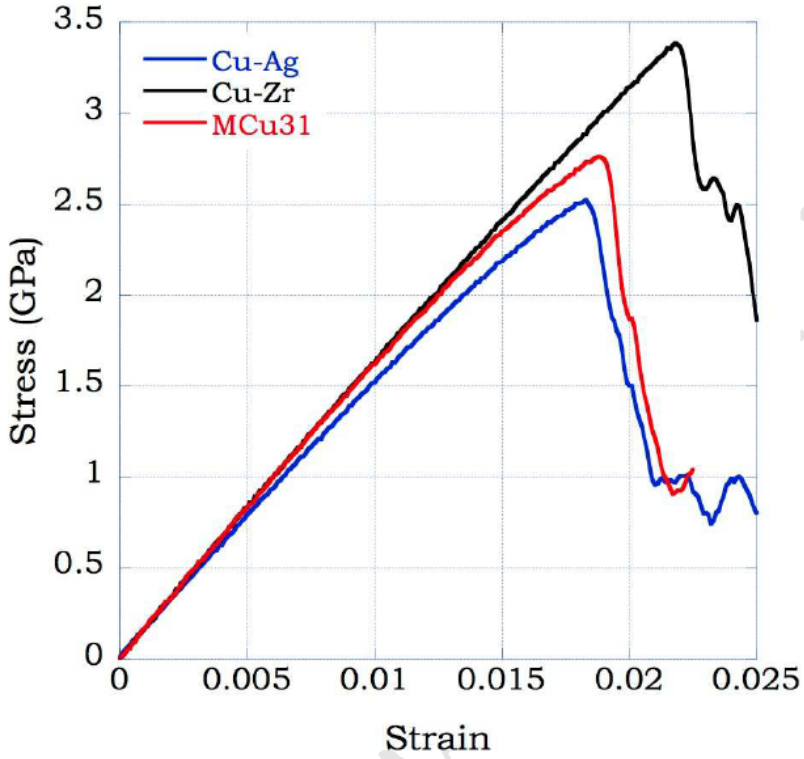

Figure 2. Stress-strain curves for the Cu potentials from (Borovikov et al., 2016; Mendelev et al., 2009; Williams et al., 2006).

Since the Cu-Zr FS potential from (Mendelev et al., 2009) has been extensively tested in MD simulations we only needed to add the Cu-Zr cross-species pair potential. The details of the potential development procedure can be found in Supplemental Material . All of the results reported in the rest of this paper were obtained using the new Cu-Zr potential, which can be found in Supplemental Material and at http://www.ctcms.nist.gov/potentials (Ercolessi and Adams, 1994)(Ercolessi and Adams, 1994).

3. Solute segregation at the grain boundary

Ag and Zr atoms are both larger than Cu atoms; therefore, they both introduce stress fields when they substitute Cu matrix atoms. However, these fields differ in more than just their magnitudes, even in the bulk. A single Ag solute atom in the bulk is under strong compression and its Cu nearest neighbors are under much smaller compression, as shown in Fig. 3a. The stress distribution around the Zr solute, shown in Fig. 3b, is more complicated: the solute itself is under tension, while the shell of Cu nearest-neighbors is under significant compression. We also note that the Ag and Zr solutes have very different dipole interaction energies in the bulk. Zr solutes have a positive dipole interaction energy, E_d = 0.29 eV, corresponding to repulsion, while the Ag solutes have a negative dipole interaction energy, E_d = -0.09 eV, corresponding to attraction.

At small concentrations, both Ag and Zr solutes segregate exclusively at the A sites of the E structural units in the Σ11(332)[110] STGB (see Figs. 3e and 3f) because these sites are

under tension as was shown in (Duparc et al., 2005). The substitution of the Cu atom by the Ag atom at the A site changes the stress sign at this site, so it is under compression when occupied by the solute. The substitution of the Cu atom by the Zr atom at the A leads to a more complex effect: the stress at the site becomes very small but the compressive stress of several atoms on the nearby plane becomes larger.

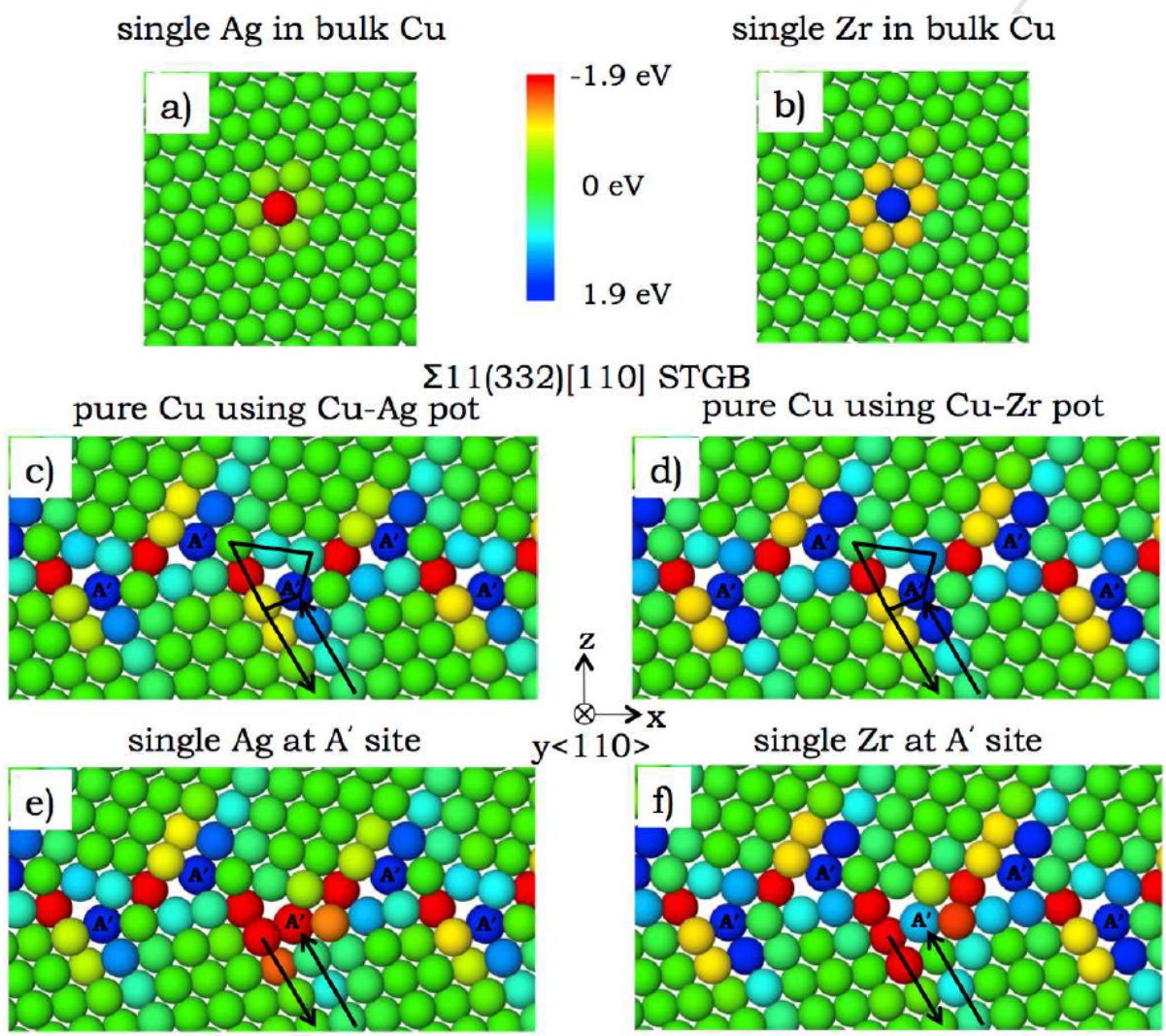

Figure 3. Distribution of stresses around: a) single Ag solute in bulk Cu; b) single Zr solute in bulk Cu; c) Σ11(332)[110] STGB, using the Cu-Ag potential; d) Σ11(332)[110] STGB, using the Cu-Zr potential; e) Σ11(332)[110] STGB with a single Ag solute at the A site; f) Σ11(332)[110] STGB with a single Zr solute at the A site. The atoms are colored according to the trace of the atomic stresses multiplied by the average atomic volume in the simulation cell. The atomic stresses were determined from the virial expressions (see (Thompson et al., 2009) for details). The arrows schematically show the direction of displacements of two atomic planes during leading partial dislocation emission from the E unit. The black polygons in c) and d) schematically indicate the E units.

The differences in segregation behavior between the Ag and Zr solutes become more pronounced at larger solute concentration. To simulate their segregation, solute atoms were introduced into the simulation cell by replacing a number of matrix (Cu) atoms in the swap regions near the grain boundaries (see Fig. 1). Next, hybrid Monte Carlo / molecular dynamics (MC/MD) simulations were carried out at T=300 K and zero applied stress, in order to obtain the equilibrium solute distribution (Sadigh et al., 2012). This simulation technique is identical to that used in (Borovikov et al., 2017). The simulation was stopped after the energy almost did not change within the last 5000000 iterations indicating that the equilibrium solute distribution was achieved (see Fig. 2 in (Borovikov et al., 2017)). We note that since equilibrium Ag or Zr concentrations in Cu are very low at T=300 K, the probability to get a solute atom in the bulk Cu in the relative small simulation cell is also very low and in fact we never observed it during the MC/MD simulation. A special simulation can be performed to find the bulk concentration corresponding to the specific GB solute concentration. Since it was not the focus of the present study, below, we will use the total solute concentration in the simulation cell which, of course, should not be confused with the equilibrium bulk concentration one can get from the phase diagram. Figure 4 shows a few representative examples of the solute distributions that we observed. At low solute concentrations (< 0.3%), both the Ag and Zr solutes segregate almost exclusively at the A sites. However, because the Zr solutes repel each other, the segregation at the A sites stops at a concentration of ~0.28%, when *every other* A site along the [110] tilt axis is filled. At higher solute concentrations, the Zr solutes segregate to other sites further away from the grain boundary. In the case of Ag solutes, segregation to the A sites continues with increasing solute concentration until *every* A site along the [110] tilt axis is filled (corresponding to an Ag solute concentration of ~0.56%). Above this concentration solute atoms begin segregating to other sites. The distribution of Ag solutes at the GB is more compact at high solute concentrations, than the corresponding distribution of the Zr solutes (see Fig. 4).

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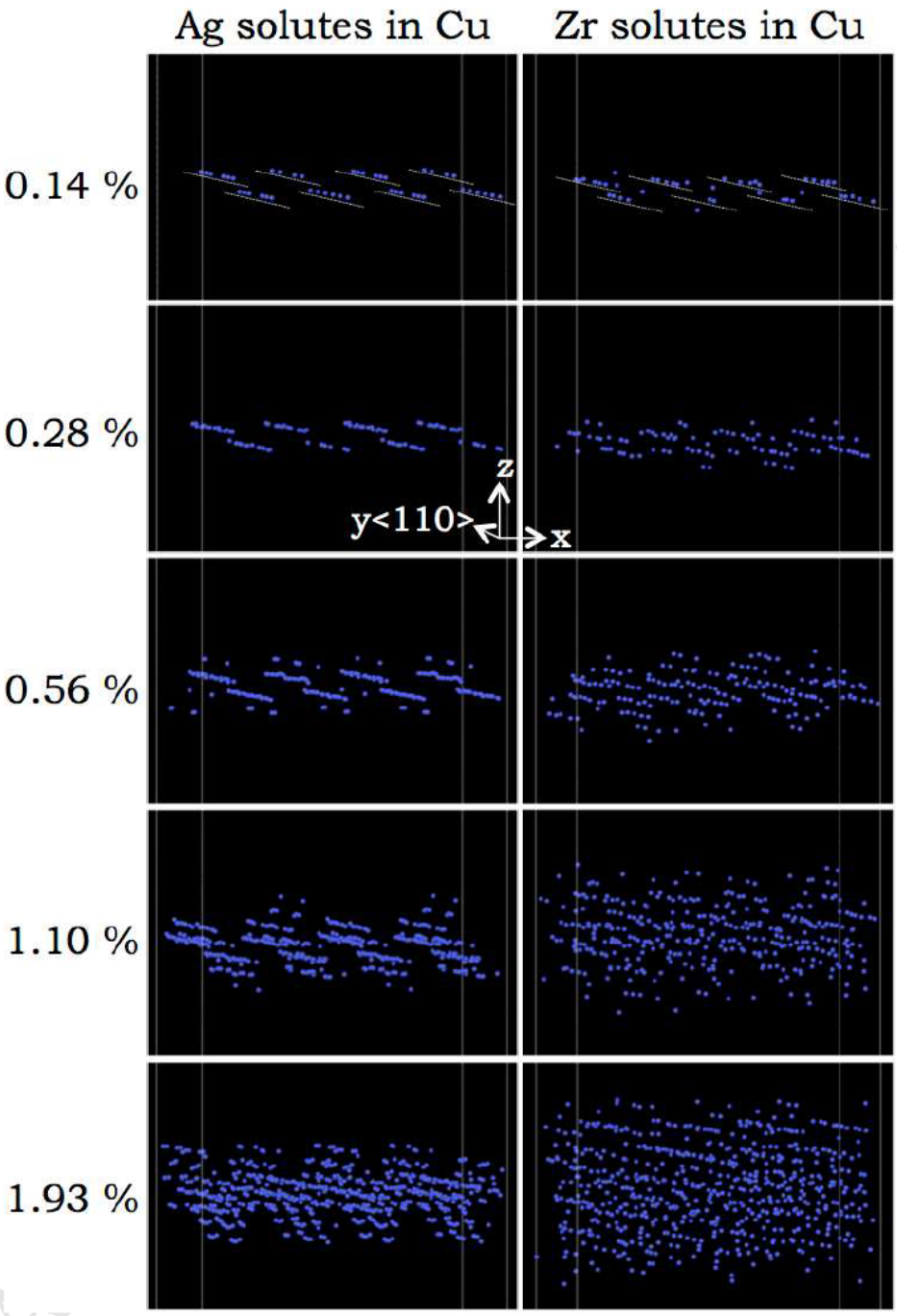

Figure 4. Representative examples of the solute distributions at Σ11(332)[110] STGB in Cu for the cases of Ag and Zr solutes. Only solute atoms are shown. Note that all Ag atoms in the left top image are segregated at the A sites (dashed lines schematically indicate the positions of the A sites).

Figure 5 shows how the addition of solutes modifies the GB structure. The effect of Ag solutes is clearly much smaller than the effect of Zr solutes. Segregating rather compactly, Ag

solutes do not appreciably change the GB structure, and the E structural units are recognizable at all concentrations. At small concentrations, the Zr solutes also do not change the GB structure but at concentrations larger than ~1.1 %, they make it much more disordered in spite of the fact that Zr solutes are more widely distributed in the direction normal to the GB than Ag solutes. The GB structure at 1.93 % Zr appears primarily amorphous with some remnants of the initial crystalline structure. This effect has been observed in both experiment and MD simulation in (Khalajhedayati et al., 2016; Khalajhedayati and Rupert, 2015; Pan and Rupert, 2016) (although the the original Cu-Zr potential from (Mendelev et al., 2009) was employed in (Pan and Rupert, 2016)).

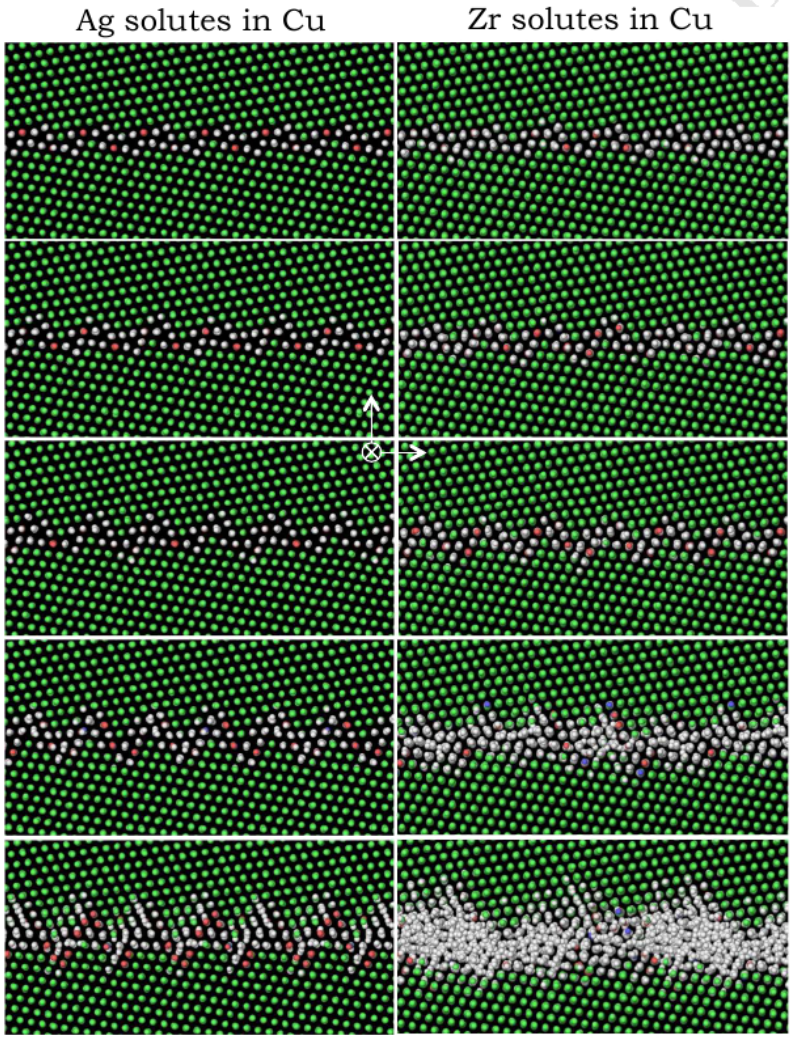

Figure 5. Disorder in the Σ11(332)[110] STGB at different solute contents. The atoms are colored according to the common neighbor analysis (CNA) (Honeycutt and Andersen, 1987; Stukowski, 2012). The color-coding is as follows: green – FCC, red – HCP, grey – others. The size of both solutes and solvents is decreased and made the same to highlight the increase in disorder with increasing solute concentration.

4. Effect of solutes on dislocation nucleation from the GB

The MD simulation of the uniaxial deformation of the simulation cells containing solutes was identical to that for pure Cu (see Section 2). Figure 6 shows the dependence of the yield stress, σ_y on the solute concentration, X, for both of the solutes considered in this study. At low concentrations, addition of either Ag or Zr increases the yield stress. In spite of the difference in the atomic mismatches for Ag and Zr, the rate of increase, $d\sigma_y/dX$, is similar for both solutes. As the concentration increases, both solutes see a drop to a lower, still positive, value of $d\sigma_y/dX$. In both cases the change of slope occurs when solute atoms begin to segregate to sites other than the A location in the grain boundary. Because Zr only occupies half of the A sites while Ag can occupy all of them, this corresponds to roughly half the concentration of Zr than it does for Ag.

At higher concentrations of Ag, the yield stress continues to increase although it fluctuates considerably after the Ag atoms substitute approximately 30% of the Cu atoms at the grain boundary (corresponding to ~0.83% total concentration). For Zr solutes, the yield stress reaches a peak when the Zr atoms substitute approximately 20% of the Cu atoms at the grain boundary (corresponding to ~0.55% total concentration), at which point $d\sigma_y/dX$ goes negative and the strengthening effect is eventually eliminated at higher Zr concentrations.

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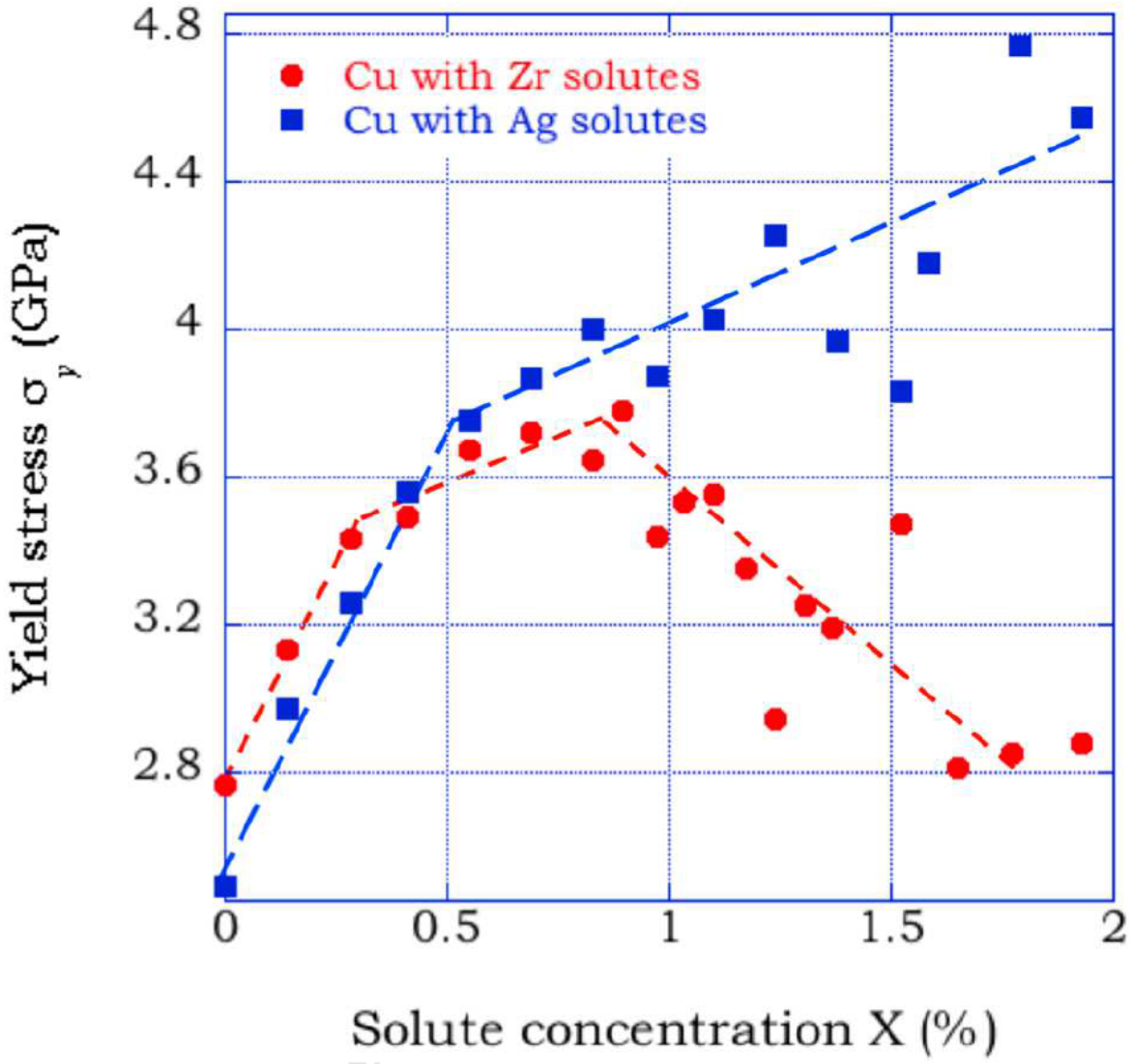

Figure 6. The dependence of the yield stress $_y$ on total solute concentration in the simulation cell(Abe et al., 2006), X (at. %). The dashed lines schematically indicate the trends observed at different solute concentrations.

These observations reveal much greater complexity than would be expected under the assumption that the tensile strength improvement should depend simply on the size mismatch of the solute. Recalling that as applied stress increases, the first dislocations are emitted from grain boundary E units (Spearot, 2008), it is possible to rationalize our findings. At small concentrations both Ag and Zr solutes segregate exclusively at the A sites of the E structural units (see Fig. 4). Dislocation emission at this location shifts the plane of atoms which includes the A site towards the E unit, while the adjacent plane which includes the atoms under compression, shifts away from the E unit (see Figs. 3c-d). The effect of Ag solutes on dislocation emission is straightforward: they change the stress at the A sites from tensile to compressive, making it more difficult for the plane of atoms which includes this site to move towards the E

unit. This increases the stress necessary for nucleation. The effect of the Zr solutes is similar: they also change the stress at the A sites. Unlike Ag solutes, however, they do not create a large compressive stress there, but they still exclude these sites from the possible locations of dislocation nucleation.

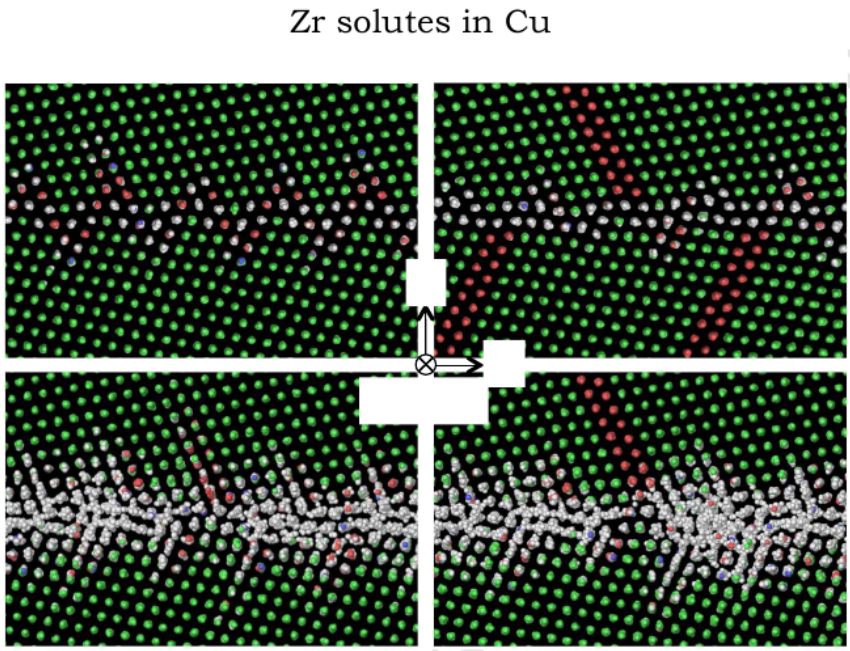

Figure 7. The change of the Σ11(332)[110] STGB structure associated with the dislocation emission. The atoms are colored according to the common neighbor analysis (CNA) (Honeycutt and Andersen, 1987; Stukowski, 2012). The color-coding is as follows: green – FCC, red – HCP, grey – others. The size of solutes and solvents is decreased and made the same to highlight the changes in the GB structure associated with the dislocation emission.

At larger Ag concentrations the solute atoms continue to segregate to the A sites, providing a continuous increase in the yield stress. However, at ~0.56 %, all A sites are occupied and the Ag solutes begin segregating at other sites (further away from the GB), which have a weaker effect on dislocation emission. This explains the change in $d\tau_y/dX_{Ag}$, clearly seen in Fig. 6. At higher concentrations, the noisy relationship between the yield stress and the Ag concentration results from the existence of multiple segregation sites that have similar segregation energies (a more detailed discussion can be found in (Borovikov et al., 2017)), and solute interactions that may lead to the formation of Ag clusters and/or Ag-Cu complexes. In this concentration regime, for Ag, there is some question whether the MC/MD method reliably finds the lowest-energy configuration among outcomes that have similar energies; and it is also possible that multiple configurations may co-exist, if they contribute sufficient configurational entropy to the Gibbs free energy of the system.

In the case of Zr, segregation to the A sites stops at a lower concentration, ~0.28%, when *every other* A site along the [110] tilt axis is filled with a solute atom. At Zr concentrations above this, the extra Zr begins to segregate to sites located further away from the GB, which have less influence on the dislocation nucleation process. This explains why $d\tau_y/dX_{Zr}$, has a

smaller value for solute concentrations between ~0.28 % and ~0.8 %. Zr concentrations increasing beyond ~0.8 % lead to the emergence and progressive enlargement of amorphous regions of the GB, producing hybrid ordered/amorphous structures like those proposed by Mott (Mott, 1948), in which the E units are the most persistent ordered regions. When a dislocation is emitted from an E unit surrounded by a periodic GB region the displacements of the atoms located near by the source are constrained, which makes it difficult to emit the dislocation. When the E units are surrounded by amorphous regions (see Fig. 7b) where displacements are not as rigidly quantized as in crystalline material, it is easier for atoms to reshuffle in order to accommodate the displacements associated with dislocation emission. Increasing amorphization with increasing Zr concentration thus reduces the yield strength for concentrations above ~0.8 %.

All results reported in the present paper were obtained using the particular semi-empirical potentials. Other semi-empirical potentials are available for the Cu-Ag-Zr alloys. For example, a Cu-Ag-Zr EAM potential was developed in (Fujita et al., 2010; Fujita et al., 2009). It would be very useful and interesting to repeat the simulations performed in the present study using this potential to investigate how the obtained results depend on the choice of a semi-empirical potential. The key quantity determining the difference between the Ag and Zr solute effects is the solute dipole interaction energy. Indeed, it is the repulsion between the Zr atoms which does not allow them to segregate at the A sites next to each other, leading to a different segregation pattern and eventual amorphization of the GB structure. Using the Cu-Ag-Zr EAM potential developed in (Fujita et al., 2010; Fujita et al., 2009) we obtained E_d = -0.005 eV for the Ag-Ag bulk dipoles and E_d = 0.14 eV for the Zr-Zr bulk dipoles. These values are somewhat different from the values obtained using the semi-empirical potential employed in the present study (-0.09 and 0.29 eV, respectively) but the trend is obviously the same. Therefore, we expect to obtain qualitatively the same results using the Cu-Ag-Zr EAM potential developed in (Fujita et al., 2010; Fujita et al., 2009).

5. Conclusions

The effects of solute segregation on dislocation emission from grain boundaries are complex, and the size misfit of a segregant with its host is not a reliable guide to its impact on the yield strength in a nanocrystalline material. Using atomistic simulations, we demonstrate that the effect of solutes on the dislocation nucleation from a grain boundary strongly depends on the equilibrium distribution of solutes at this grain boundary, which can vary dramatically depending on the solute type. In particular, we show that the solute atoms with a *smaller* size mismatch (Ag solutes in Cu) can be more effective in suppressing the dislocation emission from grain boundaries compared to the solutes with a larger size mismatch (Zr solutes in Cu). Moreover, we demonstrate that high concentrations of Zr solutes may lead to amorphization of the grain boundary and reduction of the yield stress.

While a number of recent studies have demonstrated that Zr is an excellent candidate for stabilizing nanocrystalline Cu against grain growth (Atwater et al., 2013; Khalajhedayati and Rupert, 2015; Rupert, 2016), our results indicate that it may not be very effective in suppressing dislocation emission from grain boundaries under applied stress (compared, for example, to Ag). Since the dominant mechanism of plastic deformation in nanoscale metals and alloys is dislocation slip originating from grain boundaries or their triple junctions, it may be possible to identify optimal solute additions, which serve the dual purposes of stabilizing a nanocrystalline

material against grain growth and suppressing dislocation nucleation from its grain boundaries. It remains to be determined if there is any interplay between these two functions.

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